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**From:** Sun, Meng@OEHHA [meng.sun@oehha.ca.gov]  
**Sent:** 5/13/2019 6:09:51 PM  
**To:** Williams, Antony [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=959e02b5a0da419a9d749469dfe05c34-Williams, A]; Paul-Friedman, Katie [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=9de6209426a941908301318615f5507b-Paul-Friedm]  
**Subject:** RE: Questions regarding the Chemistry Dashboard

Thank you both so much. Katie, I appreciate you going into details in explaining the situation for NVS. Tony, thank you for the heads-up on single concentration data. I think for the current hazard identification document we will utilize what the Chemicals Dashboard has to offer now to make our deadline, but please keep us posted on future updates to the Dashboard. Thank you for what you do to make NAM data accessible.

Meng

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**From:** Williams, Antony <Williams.Antony@epa.gov>  
**Sent:** Monday, May 13, 2019 9:16 AM  
**To:** Paul-Friedman, Katie <Paul-Friedman.Katie@epa.gov>; Sun, Meng@OEHHA <meng.sun@oehha.ca.gov>  
**Subject:** RE: Questions regarding the Chemistry Dashboard

Meng,

Just to let you know that we are intending to support single concentration data in a later version of the CompTox Chemicals Dashboard and Katie and I have been discussing this for a while and it is in the top priorities for future development. Best wishes.

Antony J. Williams  
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Try out the [CompTox Chemicals Dashboard](#) and access data for almost 875,000 chemical substances

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**From:** Paul-Friedman, Katie  
**Sent:** Monday, May 13, 2019 9:11 AM  
**To:** Sun, Meng@OEHHA <meng.sun@oehha.ca.gov>; Williams, Antony <Williams.Antony@epa.gov>  
**Subject:** RE: Questions regarding the Chemistry Dashboard

Hi Meng and Tony,

I wanted to provide a little input on the NVS issue for the chemical mentioned if it is of interest.

- The bug fix released last week on the CompTox Chemicals Dashboard should make the assay hit counts consistent between tabs and remedy “dropped data.”
- Though there are 63 screened NVS assays showing the ToxCast Dashboard (invitrodb version 2.0), none of them were shown as positive (which is actually in error; see more in next bullets).

- In the latest release of ToxCast (invitrodb version 3.1), it looks like 5 NVS assays are positive (out of 6 tested).
- The discrepancy in the number of tested assays appears to be how the ToxCast Dashboard and the CompTox Chemicals Dashboard are treating single concentration screening data. In invitrodb version 3.1, I can see that 63 NVS assays were tested in single concentration for NVS (that assay technology had a tiered strategy, with single concentration screening at a high concentration, followed by multi-concentration testing if warranted). In invitrodb version 3.1, 7 of the 63 single concentration screens in NVS were positive for this chemical. It appears that the ToxCast Dashboard all 63 NVS assays are showing as tested but negative. In the CompTox Chemicals Dashboard, there is currently not a utility to view single concentration screening data. So all you see there currently is the multi-concentration screening, where 6 assays were performed and 5 were positive.

Please let us know if you need any further clarification or assistance in using these information.

Thanks,

Katie

Katie Paul Friedman, PhD

Toxicologist

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**From:** Sun, Meng@OEHHA <[meng.sun@oehha.ca.gov](mailto:meng.sun@oehha.ca.gov)>

**Sent:** Friday, May 10, 2019 7:33 PM

**To:** Williams, Antony <[Williams.Antony@epa.gov](mailto:Williams.Antony@epa.gov)>

**Cc:** Paul-Friedman, Katie <[Paul-Friedman.Katie@epa.gov](mailto:Paul-Friedman.Katie@epa.gov)>

**Subject:** RE: Questions regarding the Chemistry Dashboard

Hello Antony,

Thank you so much for the detailed answers! I really appreciate you taking the time to explain these, including the slides on the recent release of invitroDBv3.1. And I now know that the proper name is the Chemicals Dashboard ☺

Regarding my questions on how to analyze the data, I guess I was asking because of the discrepancy of active calls. Now that you mentioned the background assays, I think we know what to do. I personally would not count the background assays.

Have a great weekend!

Meng

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**From:** Williams, Antony <[Williams.Antony@epa.gov](mailto:Williams.Antony@epa.gov)>

**Sent:** Friday, May 10, 2019 8:06 AM

**To:** Sun, Meng@OEHHA <[meng.sun@oehha.ca.gov](mailto:meng.sun@oehha.ca.gov)>

**Cc:** Paul-Friedman, Katie <[Paul-Friedman.Katie@epa.gov](mailto:Paul-Friedman.Katie@epa.gov)>

**Subject:** RE: Questions regarding the Chemistry Dashboard

Meng,

Thank you for your email. I have attempted a response to your questions below and cc'ed Katie Paul-Friedman who is my colleague who has worked with me to get invitroDBv3.1 into the CompTox Chemicals Dashboard (it was renamed from the Chemistry Dashboard last year).

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**From:** Sun, Meng@OEHHA [<mailto:meng.sun@oehha.ca.gov>]

**Sent:** Thursday, May 9, 2019 5:33 PM

**To:** Williams, Antony <[Williams.Antony@epa.gov](mailto:Williams.Antony@epa.gov)>

**Subject:** Questions regarding the Chemistry Dashboard

Hello Tony,

Thank you so much for agreeing to help us with your expertise on the Dashboard. As Jennifer and Elizabeth have mentioned, we are trying to use the ToxCast/Tox21 data for three chemicals, and we identified some questions during that process. I attached a figure of the assay counts for one of the three chemicals, 1,4-bq, and some questions here.

## ToxCast data for 1,4-benzoquinone: inconsistency from two data portals

- 100/556 active/total assays tested (source: ChemDashboard)
- 88/513 active/total assays tested (source: ToxCast Dashboard)

	ACEA	ATP	BSK	NVS	Tox21
Chemistry Dashboard	2	163	174	6	211
ToxCast Dashboard	0	163	174	63	113

**[AJW>] Just FYI we rolled out a new version overnight and now it is 105/556 as ACTIVE hit calls including background measurement are now included:**

105 active of 556 assays

Download Columns 10

Search Query  Show Inactive ☐ Show Background ☒

Name	Model	SeqsPKES	ADP	Event	Hit Call	Top	AC30	logAC30	MaxMed	Cutoff	ModAcc	Intended Target Family
ATQ_Amy_CIS_up		NP_001812.1	150	12	ACTIVE	4.42	2.77	0.396	1.86	0.894	-0.330	dna binding
ATQ_AP_1_CIS_up		NP_005243.1	-	-	ACTIVE	1.19	51.6	1.71	0.394	0.935	1.71	dna binding
ATQ_Oxy_CIS_up		-	-	-	ACTIVE	0.867	72.3	1.86	0.856	0.675	1.50	background measurement
ATQ_PRL_CIS_up		NP_000146.2	200	1191	ACTIVE	3.07	16.3	1.26	1.70	0.503	1.72	nuclear receptor
ATQ_HF1a_CIS_up		NP_091521.1	-	-	ACTIVE	1.10	28.9	1.48	1.09	0.773	1.50	dna binding

Our questions include:

1. Why is there a difference of assay counts for this chemical between the ToxCast Dashboard and the Chemistry Dashboard?

**[AJW>] The ToxCast dashboard is no longer being maintained and invitroDBv3.1 has been rolled out in the Chemicals Dashboard only. Katie and I presented on this recently here: <https://www.epa.gov/chemical-research/computational-toxicology-communities-practice-comptox-chemicals-dashboard-and> . It is expected that the Chemicals Dashboard will have more data than the ToxCast Dashboard. We will retire the ToxCast dashboard later in the year (around August).**

2. Does the Chemistry Dashboard absorb new Tox21 data as they become available sooner than the ToxCast Dashboard?

**[AJW>] Any new data from Tox21 will ONLY show up in the Chemicals Dashboard from this point.**

3. Does the Chemistry Dashboard take the Tox21 QC results into consideration for data analysis?

**[AJW>] When Tox21 QC data are available at the Tripod site we map and display them at the top of the page. We are building our own AnalyticalQC database with a lot more data and that will be integrated in the future.**

4. Specifically, for 1,4-benzoquinone, why is there only 6 NVS assays on the ChemDashboard, but 63 from ToxCast Dashboard?

**[AJW>] I am going to leave that one to Katie as we have received similar comments from others and it is possible that some Tox21 data have been dropped and I believe this is being investigated.**

5. What is the difference between the active calls for another chemical (4-aminophenol) from the Tox21/ToxCast tab on the Chemistry Dashboard (gives 45/211 actives) and the ToxCast summary tab (gives 94/133 actives)?

**[AJW>] The Chemicals Dashboard now gives "122 active of 211 assays" including background and 94 of 211 when background is excluded.**

How would you recommend that we do to analyze the data?

**[AJW>] Can you be more specific with the question possibly? I am not sure what question you are trying to answer?**

If it works for you, I can give you a call sometime next week at your convenience. What days and time work best for you? Thank you so much for your help.

**[AJW>] We can chat next week if these answers do not cover everything. Thanks**

Meng

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